

DE LA RECHERCHE À L'INDUSTRIE



A Lagrangian conservative space and time staggered hydrodynamic scheme

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Multimat - september 5th 2013

Present trends for Lagrange (and ALE) hydro schemes give preference to **time (and even space) centering** of all conservative quantities

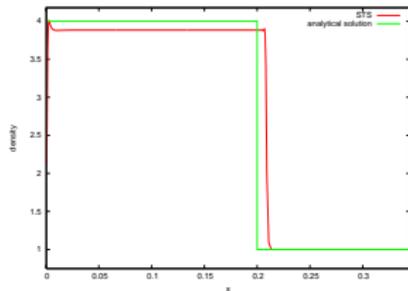
- CAVEAT scheme: [Addessio, Baugardner, Dukowicz, Johnson, Kashiwa, Rauenzahn, Zemach, 1990]
- Compatible-Hydro scheme: [Caramana, Burton, Shashkov, Whalen 1998]
- GLACE scheme: [Després, Mazeran, 2003]
- EUCCLHYD scheme: [Maire, 2004, 2007]

Notations:

“VNR” (Von Neumann–Richtmyer, 1D) \equiv “Wilkins” (2D)
 \equiv “SGH” (Staggered Grid Hydro) \equiv “STS” (Space and Time Staggered)

“CSTS” = Conservative Space and Time Staggered

Most widely known distortion: shock levels and velocities



Density profiles STS scheme on plane Noh's test:
 $\approx 5\%$ error on density jump and propagation velocity

However:

- time and space staggered schemes are extremely practical and widely used ([von Neumann–Richtmyer 1950], [Wilkins 1964], [Pracht 1975]...)
- yet, little research effort spent on such schemes (hopeless? old fashioned? focus on Q & anti-hourglassing?...)
- there is no theorem or proof that conservativity cannot be achieved
- and hints are actually that **total energy can be exactly conserved** ([Trulio & Trigger 1960], [Burton 1991])

Here, reexamine, extend, and assess conservative modified STS schemes

I. Write a modified STS scheme with following properties:

- same calculation structure as the STS (1, 2, or 3D)
- second order in time and space as the STS
- exactly conservative in mass, momentum, and total energy
- under all conditions (regardless of time step changes)
- with a kinetic energy defined by a positive definite quadratic form of velocity (rules out Trulio & Trigger's $E_c = \sum_i m_i \mathbf{u}_i^{n+1/2} \cdot \mathbf{u}_i^{n-1/2}$)
- and, if possible, second order entropic (bonus, demands energy conservation)

II. Basic tests of impact on:

- energy conservation
- jump conditions
- constraints on time step
- mesh behavior in 2D

- Continuous system of equations
- “Historical” space and time discretization
- CSTS scheme
 - Conservative Space and Time Discretization
 - Kinetic energy equation
 - Internal energy equation
 - Numerical example: Noh 1D
 - Total energy conservation
 - Rewriting of the internal energy
 - Entropy condition
 - Order one artificial viscosity
 - Order two predicted–corrected artificial viscosity
 - Numerical example: Noh 1D
 - Comments on the effective energy of the system
- Numerical results
 - Sod
 - Noh 2D
 - Kidder

- Continuous system of equations
- “Historical” space and time discretization

CSTS scheme

Conservative Space and Time Discretization

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We solve compressible Euler's equations:

$$\left\{ \begin{array}{ll} \frac{d\mathbf{x}}{dt} = \mathbf{u} & \text{semi-Lagrangian configuration} \quad (1a) \\ \frac{d\rho}{dt} = -\rho \nabla \cdot \mathbf{u} & \text{mass conservation} \quad (1b) \\ \rho \frac{d\mathbf{u}}{dt} = -\nabla(p + q) & \text{momentum conservation} \quad (1c) \\ \rho \frac{de}{dt} = -(p + q) \nabla \cdot \mathbf{u} & \text{internal energy evolution} \quad (1d) \\ p = \text{EOS}(\rho, e) & \text{system closure} \quad (1e) \end{array} \right.$$

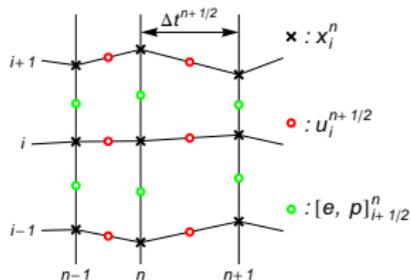
where \mathbf{u} is velocity, ρ density, p pressure, q artificial viscosity and e internal energy

System (1) writes:

$$\left\{ \begin{array}{l} \mathbf{x}_p^{n+1} = \mathbf{x}_p^n + \mathbf{u}_p^{n+1/2} \Delta t^{n+1/2} \quad (2a) \\ m_c^{n+1} = m_c^n \quad (2b) \\ m_p(\mathbf{u}_p^{n+1/2} - \mathbf{u}_p^{n-1/2}) = \sum_{c \in C(p)} (p+q)_c^n \frac{\partial V_c}{\partial \mathbf{x}_p} \Big|_n \frac{\Delta t^{n+1/2} + \Delta t^{n-1/2}}{2} \quad (2c) \\ \frac{e_c^{n+1} - e_c^n}{\Delta t^{n+1/2}} = - \frac{(p+q)_c^{n+1/2}}{\Delta t^{n+1/2}} \left(\frac{1}{\rho_c^{n+1}} - \frac{1}{\rho_c^n} \right) \quad (2d) \\ \rho_c^{n+1} = EOS(\rho_c^{n+1}, e_c^{n+1}) \quad (2e) \end{array} \right.$$

where:

- c cell labels, p node labels
- $\Delta t^{n+1/2}$ time step between t^n and t^{n+1}
- $\frac{\partial V_c}{\partial \mathbf{x}_p} \Big|_n$ corner vectors
- $\rho_c^{n+1/2} = \frac{1}{2}(\rho_c^n + \rho_c^{n+1})$
- $m_p = \sum_{c \in C(p)} \frac{1}{|C(p)|} m_c$



Continuous system of equations

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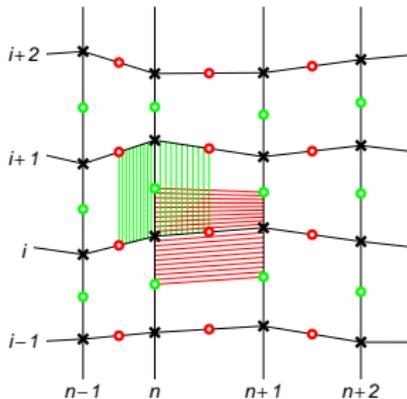
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Sod

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Kidder

Conservative Space and Time Discretization



Consistency demands that **action** \mathcal{A} (= time integral of energy) be built from kinetic and internal energies discretized over the **STS grid**:

$$E_i^n = \sum_c m_c e_c^n$$

$$E_k^{n+1/2} = \sum_p \frac{1}{2} m_p (\mathbf{u}_p^{n+1/2})^2$$

$$\mathcal{A} = \sum_n \frac{1}{2} (\Delta t^{n-1/2} + \Delta t^{n+1/2}) E_i^n + \Delta t^{n-1/2} E_k^{n-1/2}$$

- This is a form of “space-time finite volumes approach” (second-order accurate)
- A least action variational principle yields the **only possible** momentum equation: turns out be identical to the original STS scheme
- Now, from there, total energy conservation can be **deduced** so as to be compatible with the discretization of action: turns out there is **only one possible scheme** (for the given formula of E_k)

Kinetic energy equation

The **momentum equation**:

$$m_p(\mathbf{u}_p^{n+1/2} - \mathbf{u}_p^{n-1/2}) = \sum_{c \in C(p)} (\rho + q)_c^n \frac{\partial V_c}{\partial \mathbf{x}_p} \Big|_c \frac{\Delta t^{n+1/2} + \Delta t^{n-1/2}}{2}$$

multiplied by $\frac{1}{2} (\mathbf{u}_p^{n+1/2} + \mathbf{u}_p^{n-1/2})$, we obtain the **kinetic energy equation**:

$$\begin{aligned} & \frac{1}{2} m_p [(\mathbf{u}_p^{n+1/2})^2 - (\mathbf{u}_p^{n-1/2})^2] \\ &= \sum_{c \in C(p)} (\rho + q)_c^n \frac{\partial V_c}{\partial \mathbf{x}_p} \Big|_c \cdot \frac{\mathbf{u}_p^{n+1/2} + \mathbf{u}_p^{n-1/2}}{2} \frac{\Delta t^{n+1/2} + \Delta t^{n-1/2}}{2} \quad (3) \end{aligned}$$

Internal energy equation

We use the same “energy tally” argument as [Burton, 91]:

- internal energy equation must **match** the kinetic energy equation
→ **only flux terms are left**
- right hand sides of kinetic and internal energies must be opposite up to both **space and time index rearrangements**

$$\begin{aligned}
 m_c(e_c^{n+1} - e_c^n) &= \sum_{p \in P(c)} -\frac{1}{2} \left[(p+q)_c^{n+1} \frac{\partial V_c}{\partial \mathbf{x}_p} \Big|^{n+1} + (p+q)_c^n \frac{\partial V_c}{\partial \mathbf{x}_p} \Big|^n \right] \cdot \mathbf{u}_p^{n+1/2} \Delta t^{n+1/2} \\
 &\quad + \frac{1}{4} (p+q)_c^n \frac{\partial V_c}{\partial \mathbf{x}_p} \Big|^n \cdot (\mathbf{u}_p^{n+1/2} - \mathbf{u}_p^{n-1/2}) (\Delta t^{n+1/2} - \Delta t^{n-1/2}) \quad (4)
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 &\quad \text{second order accuracy in time} \\
 &\quad + \frac{1}{4} (p+q)_c^n \frac{\partial V_c}{\partial x_p} \Big|^n \cdot (\mathbf{u}_p^{n+1/2} - \mathbf{u}_p^{n-1/2}) (\Delta t^{n+1/2} - \Delta t^{n-1/2}) \quad (4)
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 \end{aligned}$$

- rearrangement of the remaining terms of (3)
- compatible with causality: no time indices beyond $n+1$
- small and cancels for constant Δt

The internal energy equation (4) differs from its version in the STS schemes by 3 important features:

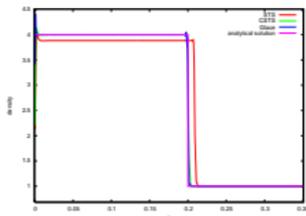
- **artificial viscosity** is now **time centered** as pressure (previously suggested by [Trulio & Trigger, 62])
- the volume variations which produce the pressure work are described by the **scalar products of corner vectors and displacements**: $\frac{\partial V_c}{\partial x_p} \cdot \mathbf{u}_p$
- a novel **corrective term** is required when the time step fluctuates

Moreover, there is a minor additional computational time.

Numerical example: plane 1D Noh's test case

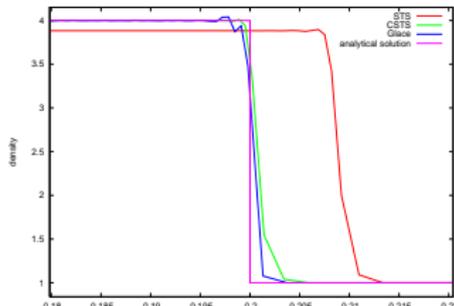
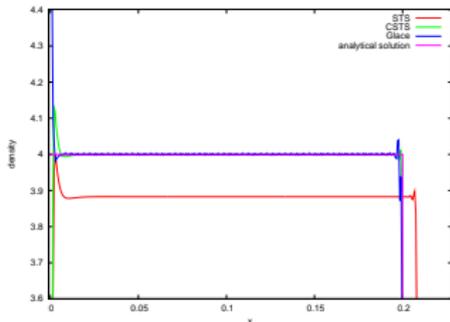
Comparison between: **STS**, **CSTS** and **cell-centered** (GLACE order 2) schemes

Density profiles at final time $t = 0.6$, CFL= 0.5



better shock level

better shock propagation velocity



Total energy conservation

Adding (3) and (4) and summing over cells and nodes yields

$$\begin{aligned} \sum_p \frac{1}{2} m_p \left[(\mathbf{u}_p^{n+1/2})^2 - (\mathbf{u}_p^{n-1/2})^2 \right] + \sum_c m_c (e_c^{n+1} - e_c^n) \\ = \sum_P \sum_{c \in C(p)} -\frac{1}{2} \left[(\rho + q)_c^{n+1} \frac{\partial V_c}{\partial \mathbf{x}_p} \Big|^{n+1} \cdot \mathbf{u}_p^{n+1/2} \Delta t^{n+1/2} \right. \\ \left. - (\rho + q)_c^n \frac{\partial V_c}{\partial \mathbf{x}_p} \Big|^n \cdot \mathbf{u}_p^{n-1/2} \Delta t^{n-1/2} \right] \end{aligned}$$

where the right hand side appears to be a **flux term in time**

Total energy conservation

The conserved numerical energy can thus be written as:

$$E_{\text{Tot.}}^{n-1/2} = E_{\text{Kin.}}^{n-1/2} + E_{\text{Int.}}^{n-1/2} = \sum_p \frac{1}{2} m_p (\mathbf{u}_p^{n-1/2})^2 + \sum_c \left[m_c e_c^n + (p + q)_c^n \sum_{p \in P(c)} \frac{\partial V_c}{\partial \mathbf{x}_p} \Big|_c^n \cdot \mathbf{u}_p^{n-1/2} \frac{\Delta t^{n-1/2}}{2} \right]$$

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 &+ \sum_c \left[m_c e_c^n + (p + q)_c^n \sum_{p \in P(c)} \frac{\partial V_c}{\partial \mathbf{x}_p} \Big|_c^n \cdot \mathbf{u}_p^{n-1/2} \frac{\Delta t^{n-1/2}}{2} \right]
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internal energy backward reconstructed at $t^{n-1/2}$

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internal energy backward reconstructed at $t^{n-1/2}$

or

$$E_{\text{Tot.}}^{n-1/2} = E_{\text{Tot.}}^n = E_{\text{Kin.}}^n + E_{\text{Int.}}^n = \sum_c m_c e_c^n$$

$$+ \sum_p \left[\frac{1}{2} m_p (\mathbf{u}_p^{n-1/2})^2 + \mathbf{u}_p^{n-1/2} \cdot \sum_{c \in C(p)} (\rho + q)_c^n \frac{\partial V_c}{\partial \mathbf{x}_p} \Big|_c^n \frac{\Delta t^{n-1/2}}{2} \right]$$

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internal energy backward reconstructed at $t^{n-1/2}$

or

$$E_{\text{Tot.}}^{n-1/2} = E_{\text{Tot.}}^n = E_{\text{Kin.}}^n + E_{\text{Int.}}^n = \sum_c m_c e_c^n$$

$$+ \sum_p \left[\frac{1}{2} m_p (\mathbf{u}_p^{n-1/2})^2 + \mathbf{u}_p^{n-1/2} \cdot \sum_{c \in C(p)} (p+q)_c^n \frac{\partial V_c}{\partial \mathbf{x}_p} \Big|_c^n \frac{\Delta t^{n-1/2}}{2} \right]$$

- non positive definite quadratic form

- kinetic energy forward reconstructed at t^n

Total energy conservation

The conserved numerical energy can thus be written as:

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$$+ \sum_c \left[m_c e_c^n + (p+q)_c^n \sum_{p \in P(c)} \frac{\partial V_c}{\partial \mathbf{x}_p} \Big| ^n \cdot \mathbf{u}_p^{n-1/2} \frac{\Delta t^{n-1/2}}{2} \right]$$

internal energy backward reconstructed at $t^{n-1/2}$

- internal energy, backward reconstructed to half-integer time indices

$$m_c e_c^{n-1/2} = m_c e_c^n + (p+q)_c^n \sum_{p \in P(c)} \frac{\partial V_c}{\partial \mathbf{x}_p} \Big| ^n \cdot \mathbf{u}_p^{n-1/2} \frac{\Delta t^{n-1/2}}{2}$$

- evolution equation of internal energy:

$$m_c (e_c^{n+1/2} - e_c^{n-1/2}) = \sum_{p \in P(c)} -(p+q)_c^n \frac{\partial V_c}{\partial \mathbf{x}_p} \Big| ^n \cdot \frac{(\mathbf{u}_p^{n+1/2} + \mathbf{u}_p^{n-1/2})}{2} \frac{(\Delta t^{n+1/2} + \Delta t^{n-1/2})}{2}$$

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Order one artificial viscosity

From internal energy evolution equation of $e_c^{n-1/2}$, **entropy condition** $de + pdV > 0$ becomes

$$-q_c^n \sum_{p \in P(c)} \frac{\partial V_c}{\partial x_p} \Big| ^n \cdot \frac{(\mathbf{u}_p^{n+1/2} + \mathbf{u}_p^{n-1/2})}{2} \geq 0 \quad \text{for any cell } c$$

→ order two and **implicit**

Order one in time approximation (usual STS schemes):

q_c^n will be an explicit clipped functional of $\{\mathbf{u}_p^{n-1/2}\}$, instead of $\{\frac{1}{2}(\mathbf{u}_p^{n+1/2} + \mathbf{u}_p^{n-1/2})\}$

$$q_c^n = \underline{Q}_c(\{\mathbf{u}_p^{n-1/2}\}) = \begin{cases} Q_c(\{\mathbf{u}_p^{n-1/2}\}) & \text{if } Q_c(\{\mathbf{u}_p^{n-1/2}\}) \sum_{p \in P(c)} \frac{\partial V_c}{\partial x_p} \Big| ^n \cdot \mathbf{u}_p^{n-1/2} < 0 \\ 0 & \text{if } Q_c(\{\mathbf{u}_p^{n-1/2}\}) \sum_{p \in P(c)} \frac{\partial V_c}{\partial x_p} \Big| ^n \cdot \mathbf{u}_p^{n-1/2} \geq 0 \end{cases}$$

Q_c can be any convenient sensible formula (scalar, tensor, TVD, hyper-viscous...)

Order two predicted–corrected artificial viscosity

- **no guarantee** that order one explicit q complies with entropy condition
- what about **singularities** and large (variable) Δt ?
- significant improvement can be obtained with **predicted–corrected** q which requires **computing the momentum equation twice**:

$$m_p(\mathbf{u}_p^{*n+1/2} - \mathbf{u}_p^{n-1/2}) = \sum_{c \in C(p)} (p_c^n + q_c^{n-1/2}) \frac{\partial V_c}{\partial \mathbf{x}_p} \Big|_n \frac{\Delta t^{n+1/2} + \Delta t^{n-1/2}}{2}$$

where $q_c^{n-1/2} = \underline{Q}_c(\{\mathbf{u}_p^{n-1/2}\})$ predicted (5a)

$$m_p(\mathbf{u}_p^{n+1/2} - \mathbf{u}_p^{n-1/2}) = \sum_{c \in C(p)} (p_c^n + q_c^n) \frac{\partial V_c}{\partial \mathbf{x}_p} \Big|_n \frac{\Delta t^{n+1/2} + \Delta t^{n-1/2}}{2}$$

where $q_c^n = \underline{Q}_c(\{\frac{1}{2}(\mathbf{u}_p^{*n+1/2} + \mathbf{u}_p^{n-1/2})\})$ corrected (5b)

Order two predicted–corrected artificial viscosity

- to preserve energy conservation a correction in the e_c^n equation is required

$$\begin{aligned}
 m_c(e_c^{n+1} - e_c^n) &= \sum_{p \in P(c)} -\frac{1}{2} \left[(p_c^{n+1} + q_c^{n+1/2}) \frac{\partial V_c}{\partial x_p} \Big|^{n+1} + (p + q)_c^n \frac{\partial V_c}{\partial x_p} \Big|^n \right] \cdot \mathbf{u}_p^{n+1/2} \Delta t^{n+1/2} \\
 &\quad - \frac{1}{2} (q_c^n - q_c^{n-1/2}) \frac{\partial V_c}{\partial x_p} \Big|^n \cdot \mathbf{u}_p^{n-1/2} \Delta t^{n-1/2} \\
 &\quad + \frac{1}{4} (p + q)_c^n \frac{\partial V_c}{\partial x_p} \Big|^n \cdot (\mathbf{u}_p^{n+1/2} - \mathbf{u}_p^{n-1/2}) (\Delta t^{n+1/2} - \Delta t^{n-1/2}) \quad (6)
 \end{aligned}$$

The e_c^{n+1} expression now does not involve q_c^{n+1} (replaced by available $q_c^{n+1/2}$).

- in this case, $e_c^{n-1/2}$ equation is not modified since this equation uses only corrected q

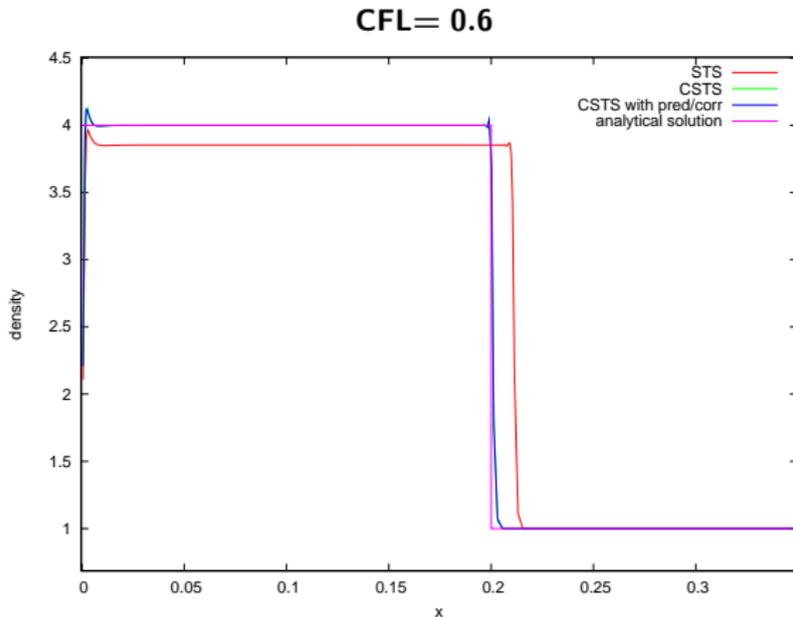
$$m_c(e_c^{n+1/2} - e_c^{n-1/2}) = \sum_{p \in P(c)} -(p_c^n + q_c^n) \frac{\partial V_c}{\partial x_p} \Big|^n \cdot \frac{(\mathbf{u}_p^{n+1/2} + \mathbf{u}_p^{n-1/2})}{2} \frac{(\Delta t^{n+1/2} + \Delta t^{n-1/2})}{2}$$

This **CSTS scheme** (5) and (6) (with predicted-corrected artificial viscosity) is now:

- **fully conservative** in momentum and total energy
- **second-order accurate** in entropy production, and
- retains the **locally implicit structure** of original STS schemes (VNR or Wilkins)

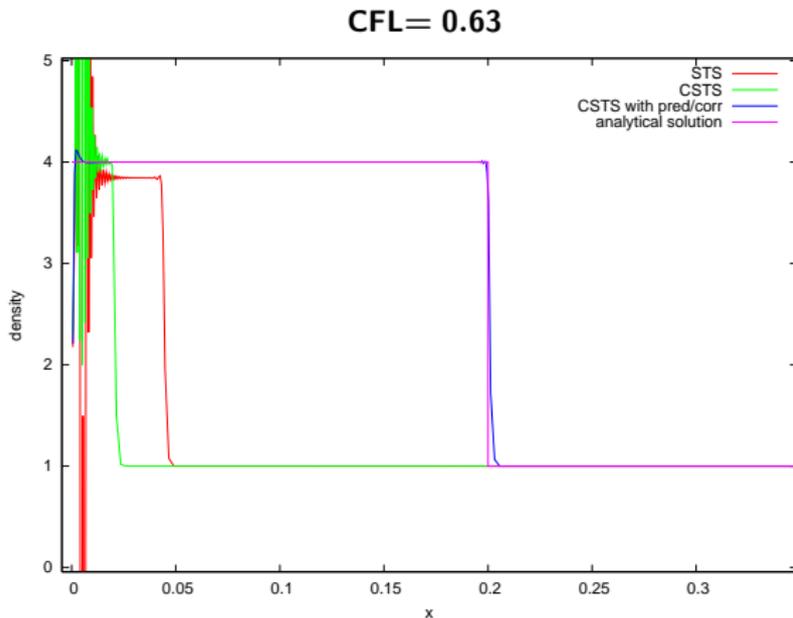
Numerical example: plane 1D Noh's test case

Influence of CFL coefficient on STS and CSTS (**without** and **with** pred-corr q):



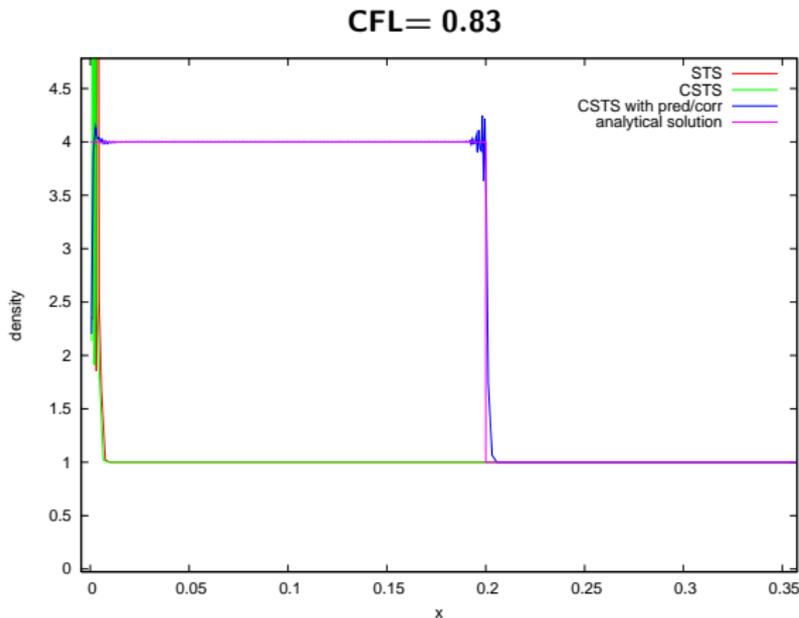
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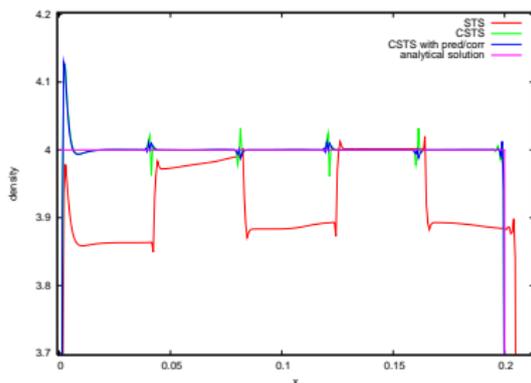
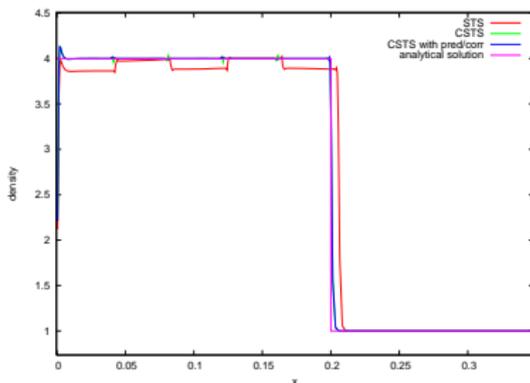
Influence of CFL coefficient on STS and CSTS (**without** and **with** pred-corr q):



Numerical example: plane 1D Noh's test case

Influence of CFL coefficient on STS and CSTS (without and with pred-corr q):

Variable CFL (0.5 and 0.1)



Continuous system of equations

"Historical" space and time discretization

- **CSTS scheme**

 - Conservative Space and Time Discretization

 - Kinetic energy equation

 - Internal energy equation

 - Numerical example: Noh 1D

 - Total energy conservation

 - Rewriting of the internal energy

 - Entropy condition

 - Order one artificial viscosity

 - Order two predicted-corrected artificial viscosity

 - Numerical example: Noh 1D

- **Comments on the effective energy of the system**

Numerical results

 - Sod

 - Noh 2D

 - Kidder

e_c^n on one hand:

- is effectively calculated by the scheme
- is used for pressure calculation (EOS)
- is not associated with a positive quadratic form of kinetic energy
- does not enforce entropic conditions

$e_c^{n-1/2}$ on the other hand:

- is not calculated by the scheme
- is not used for pressure calculation (EOS)
- is associated with a positive quadratic form of kinetic energy
- does enforce entropic conditions

Both definitions are consistent up to the accuracy order of the scheme:

$$e = e_c^n + \mathcal{O}(\Delta x^2) = e_c^{n-1/2} + \mathcal{O}(\Delta x^2) \text{ at given CFL condition}$$

Continuous system of equations

“Historical” space and time discretization

CSTS scheme

Conservative Space and Time Discretization

Kinetic energy equation

Internal energy equation

Numerical example: Noh 1D

Total energy conservation

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Numerical example: Noh 1D

Comments on the effective energy of the system

- Numerical results

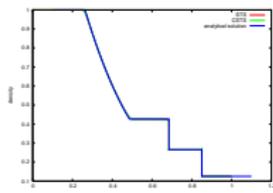
- Sod
- Noh 2D
- Kidder

Generalities

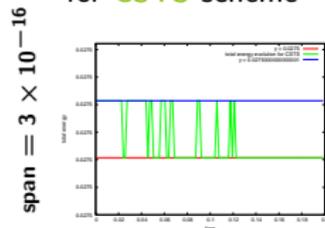
- From now on, all results for CSTS scheme use **predicted–corrected** artificial viscosity
- **Linear** artificial viscosity active in both expansion and compression: $q_1 = 0.5$
- **Quadratic** artificial viscosity active in compression only: $q_2 = \frac{\gamma+1}{4}$

SOD's test case: mesh $[5000 \times 2]$

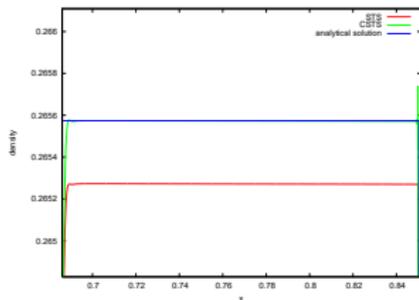
Density profiles at final time $t = 0.2$, CFL = 0.25
(**STS** and **CSTS** schemes)



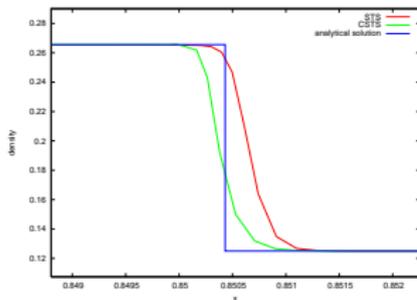
Evolution of total energy for **CSTS** scheme



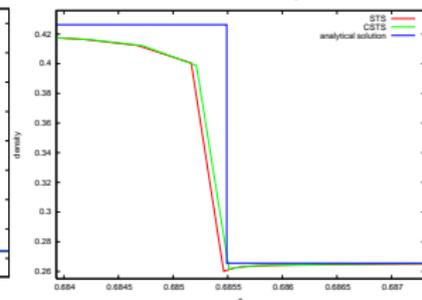
Post shock region



Shock profile



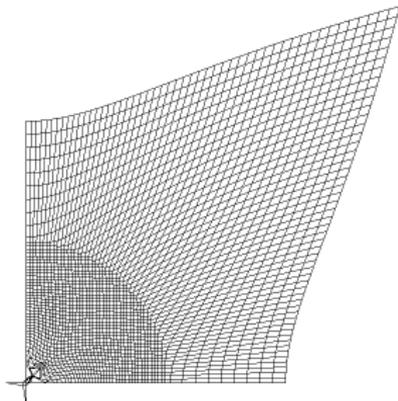
Profile of the contact discontinuity



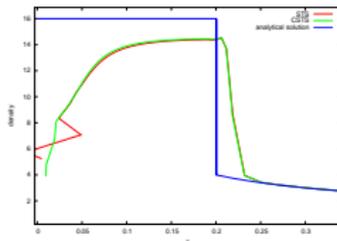
Noh's test case: 2D cylindrical

- cartesian mesh
- $\rho = 1, p = 10^{-15}, \gamma = \frac{5}{3}$
- CFL= 0.1
- no anti-hourglassing algorithm
- q 's length scale \equiv width of inertia ellipsoid along radius

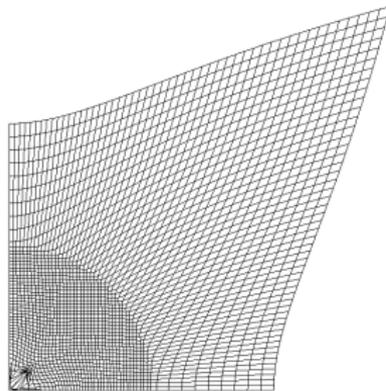
Final mesh for **STS** scheme



Density profiles at final time $t = 0.6$

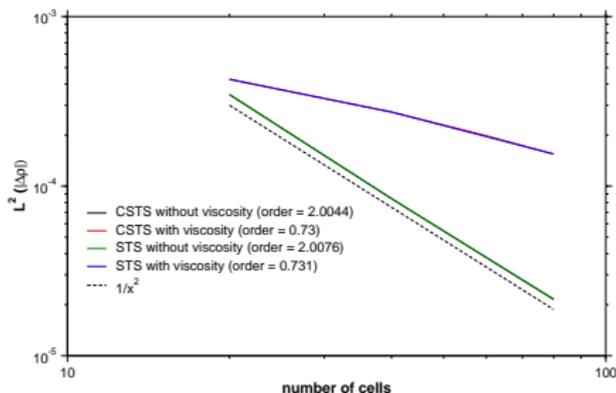


Final mesh for **CST5** scheme



Kidder's test case

Computation of the scheme's order on the density profile



3 meshes:
[20 × 20], [40 × 40], [80 × 80]

$$E_{L_2}(\rho) = \sqrt{\sum_c \Delta\rho^2}$$

$$\Delta\rho = (\rho_{theo} - \rho_{exp})$$

Conclusion

The CSTS scheme is:

- **conservative** for total energy
- **only possible** extension of usual STS schemes
- **second order** for the entropy condition

Simple numerical tests show:

- **better shock capture** (level and propagation)
- **improved 2D robustness**
- **improved CFL margin**
- reduced additional computational time: here 1% and 28% (without and with pred/corr, no Newton on EOS)

Current works

- to be submitted soon
- stability (CFL) analysis
- tests on complex EOS (shock separations...)
- other physics and numerics: ALE, 2D axisymmetric, elasticity, chemical reaction...

Acknowledgments

P. Le Tallec